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Acne, bronchitis, pink eye, ear infections, and sexually transmitted diseases are just a few of the illnesses treatable by antibiotics — assuming that the bacteria that cause these illnesses are not resistant to antibiotics.

Antibiotic resistance, one of the most urgent threats to public health, occurs when antibiotics are unable to kill the bacteria causing an infection. According to the Centers for Disease Control, each year in the United States at least 2 million people become infected with bacteria that are resistant to antibiotics and at least 23,000 people die as a direct result of these infections. Understanding antibiotic resistance starts with understanding bacteria. Bacteria are tiny single-celled organisms found nearly everywhere on Earth. Most bacteria are harmless to humans. Some are helpful. Some cause disease. Over millennia, bacteria have evolved ways to keep out harmful foreign substances. Many so-called Gram-negative bacteria, which have two cellular membranes, have evolved protein structures called efflux pumps that are lodged between the membranes and expel toxins out of the cell.

One type of efflux pump, which until recently had only been studied piecemeal, was modeled in its entirety and simulated using supercomputers at Los Alamos National Laboratory. The work harnessed the Laboratory’s extensive modeling and supercomputing simulation capabilities developed in support of its national security mission.

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